High Throughput Computing at NERSC and Beyond

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Photo: Michael Wolf, Mother Jones Magazine
3D Map of the Universe

Current Generation
– 2.5M galaxies, 2600 jobs, 50k CPU-hours

Next Generation
– 25M galaxies, 100k (?) jobs, 10M CPU-hours

How to adapt this workflow to NERSC-level supercomputers?
Common Problem: #tasks >> #jobs

Solutions tend to be...

- One-off solutions for single projects, or
- Overly complex, or
- Too simple

Those aren’t bad solutions

- e.g. PanDA, taskfarmer

They just don’t quite fill the right niche

- David Skinner: “Tactical High Throughput Computing”
- Lightweight & flexible to deploy, setup, teardown
- In the spirit of Unix command line tools
  - toolkit to build what you need
  - not monolithic Swiss army knife workflow app
- Human performance/scaling is part of the optimization
High Throughput Computing LDRD

BOSS / DESI
Flagship DOE cosmology survey studying Dark Energy:
Millions of spectra

Protein Atlas
Mapping and understanding proteins within the cell:
Millions of images

Materials Project
Simulating next-gen materials to address energy needs:
Many thousands of simulations

3 Examples / 3 Divisions
there are many more

Need NERSC-scale resources to process 1k–1M tasks
User Requirements

Scaling
- Load ~1000 tasks/second, up to ~1M tasks per workflow
- Minimal overhead when processing >10 minute tasks
- ~1000 simultaneous workflows
- ~1000 simultaneous workers each [in progress]

Features
- Dependencies & priorities between tasks
- Python + command line (Goal: REST API)
- Parallelism within tasks [in progress]

Usability
- Easy to deploy and use
- Integrates with existing clusters & super-computers
Developed by Anubhav Jain, Materials Project
– Mature, full featured, battle tested

Try same workflows on both
– possible? easy? fast?
– already good enough?
Fix bottlenecks for both
Add features to qdo

https://bitbucket.org/berkeleylab/qdo

Developed by SB, BOSS/DESI
– The scrappy young upstart
– Focus on simplicity, flexibility
Goal for qdo

If it is possible with qdo, then it is easier with qdo than anything else

Not easier?
- Let me know why
- This is a high priority for qdo

Not possible?
- Let me know why
- But no promises
  - I would rather have 80% of cases be easy than 100% of cases be possible
qdo Model

User → TaskQueue O(million) → Job(s) O(1) → Success, Failure

- Request Task
- Get Task
- Rerun everything
- Retry Failures

err = 0
err ≠ 0
Key Features

- # tasks >> # batch jobs
- Flexibility
  - Scale up/down # workers
  - Add tasks after jobs have started
- Robustness[*]
  - Queue independent of job & task failures
  - Retry just the failures
- Manage tasks in aggregate
  - Progress stats while workers are running
  - Only deal with an individual task if something went wrong with it
Real world example

#- Create a queue
import qdo
q = qdo.create(“extract”)

#- Make groups of commands to run
for group in range(32):
    commands = list()
    for i in range(25):
        commands.append(“extract {} {}”“.format(group, i))

#- Add commands to queue
ids = q.add_multiple(commands)
qu.add(“merge ”+str(g), requires=ids)

#- Launch 50 jobs to process the 832 tasks
q.launch(50)
Real world example

`#- Check status: command line interface
#- (same info available via python interface)`

```
[sbailey]$ qdo list
QueueName       State  Waiting  Pending  Running  Succeeded  Failed
extract         Active   0       0       0       826       6
```

`#- 6 Failed!?! Which ones?`
```
[sbailey]$ qdo tasks extract --state Failed
State   Task
FAILED  extract 3 18
FAILED  merge 3
...
```

`#- Debug, fix some stuff, then rerun just the failed tasks`

```
[sbailey]$ qdo retry extract
6 tasks reset to pending
```
```
[sbailey]$ qdo launch extract 3
...
```
# Load 1000 tasks
import qdo
q = qdo.create('Analyze')
for i in range(1000):
    q.add('analyze -n ' + str(i))
q.launch(10)

# after awhile (even from another process)
q.add('calibrate blat.dat', priority=100)
Advanced: params instead of execs

#- Can add any JSON-able object
q.add( dict(a=1, b=2) )
q.add( dict(a=3, b=4) )
q.add( dict(a=5, b=6) )

#- Pass in a template script to be expanded with options
q.launch(1, script="analyze -a {a} -b {b}")

#- Or pass in a function that takes task as input
def func(params):
    result = params['a'] + params['b']
    print "a+b = {}".format(result)

q.do(func=func)
Roadmap

Deploy to other users
- Get others to try it. Does it “stick”?

Web interface
- REST API + Webpage GUI

Robustness
- orphaned “running” jobs if batch job hits wallclock limit
- optional auto-retry of “random” failures

Performance tuning

Features
- dependencies: required to finish vs. required to succeed
- parallel tasks
- easier stdout/stderr log management
Summary

Tactical high throughput computing
- So easy you don’t need an expert to help you write your workflow
- qdo enables O(1M) tasks within standard batch job framework

Metric for workflow tools
- What fraction of user’s mental energy is spent on workflow vs. underlying algorithms?

Getting qdo
- https://bitbucket.org/berkeleylab/qdo
- At NERSC

```
module use /project/projectdirs/cosmo/software/modules/carver/
module load qdo/0.5
qdo --help
pydoc qdo
```

[Hopper & Edison coming soon]
Backup Slides
Efficient Queuing

HTC jobs can be flexible in shape

- Currently user has to pick both width and length
- Could just specify area and constraints instead
- Let system pick the most efficient packing

**Auto-optimize:**
- Easier for user
- More efficient for overall queue
- Easier said than done, i.e. R&D problem
Example: run a single command

#- Command line
qdo add Blat “analyze blat.dat”  #- creates queue & adds cmd
qdo launch Blat 1               #- launches 1 batch job

#- Python
import qdo
q = qdo.create(“Blat”)         #- creates queue
q.add(“analyze blat.dat”)      #- adds command
q.launch()                     #- launches 1 batch job
Example: run multiple commands

#- Command line
qdo load Blat commands.txt     #- loads file with commands
qdo launch Blat 24 --pack      #- 1 batch job; 24 mpi workers

#- Python
import qdo
q = qdo.create(“Blat”)
for i in range(1000):
    q.add(“analyze blat{}.dat”.format(i))
q.launch(24, pack=True)

#- Python load 1M tasks
commands = list()
for x in range(1000):
    for y in range(1000):
        commands.append(“analyze -x {} -y {}”\format(x, y))
q.add_multiple(commands)  #- takes ~2 minutes
q.launch(1024, pack=True)
Example: what queues exist?

#- Command line
qdo list

<table>
<thead>
<tr>
<th>QueueName</th>
<th>State</th>
<th>Waiting</th>
<th>Pending</th>
<th>Running</th>
<th>Succeeded</th>
<th>Failed</th>
</tr>
</thead>
<tbody>
<tr>
<td>BlatFoo</td>
<td>Active</td>
<td>0</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>EchoChamber</td>
<td>Active</td>
<td>0</td>
<td>46</td>
<td>0</td>
<td>50</td>
<td>4</td>
</tr>
</tbody>
</table>

#- Python
qdo.qlist()
[qdo.Queue BlatFoo at 0x1087cc790>,
 qdo.Queue EchoChamber at 0x1087cc810>]

print qdo.qlist()[0]
BlatFoo is Active
Waiting : 0
Pending : 3
Running : 0
Succeeded : 0
Failed : 0
Example: check status

```bash
#- Command line
qdo status EchoChamber
EchoChamber is Active
Waiting    : 0
Pending    : 46
Running    : 0
Succeeded  : 50
Failed     : 4

qdo tasks EchoChamber
qdo tasks EchoChamber --state=Failed
State        Task
Failed       echo 13 && sleep 1
Failed       echo 15 && sleep 1
Failed       echo 19 && sleep 1
Failed       echo 29 && sleep 1
(they failed b/c I killed them while running)
```

```python
#- Python
q = qdo.connect("EchoChamber")
q.status()
{'name': 'EchoChamber',
 'ntasks': {'Failed': 4,
            'Pending': 46,
            'Running': 0,
            'Succeeded': 50,
            'Waiting': 0},
 'state': u'Active',
 'user': 'sbailey'}

#- list of dicts of tasks
q.tasks(state='Failed')
```
Example: dependencies

```python
import qdo
q = qdo.create('MapReduce')
commands = ['echo hello '+str(i) for i in range(10)]

#- Adding commands returns list of task IDs
taskids = q.add_multiple(commands)

#- Use that list to set dependencies
q.add('echo goodbye', requires=taskids)
```
Example: retry, rerun, recover

```python
import qdo
q = qdo.connect('Blat')

#- Retry just the failed tasks
q.retry()

#- Rerun everything
q.rerun()

#- Recover from failed jobs leaving “running” tasks behind
q.recover()

#- Same thing from command line
qdo retry Blat
qdo rerun Blat --force  #- requires “--force” for safety
qdo recover Blat
```